

Dynamics of short one-dimensional nonlinear thermostated atomic chains

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Abstract

The dynamics of short 1D nonlinear Hamiltonian chains is analyzed numerically at different temperatures (energy per particle). The boundary temperature T_b separating the regular (quasiperiodic) and the stochastic (chaotic) chain motion is found. The dynamical properties of short 1D nonlinear chains interacting with thermostats are studied. It is shown that, in spite of the fluctuations, the dynamics of such systems can be stochastic as well as regular. The boundary temperature of these systems is close to that of the Hamiltonian one.

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I. INTRODUCTION

Fermi et. al [1] (FPU) were first who began to study numerically statistical properties of nonlinear 1D atomic chains. The reason for the failure of their attempt to get the redistribution of the energy of one mode between others due to nonlinearity now is clear [2].

Kolmogorov [3], Arnol'd [4] and Moser [5] (KAM theorem) have proved that in the case of small nonintegrable addition term to integrable Hamiltonian the system under some conditions can hold quasiperiodic motion on an invariant torus. Izrailev and Chirikov [6] supposed that there is the border of stochasticity for nonlinear chains. They used the resonance overlap criterion and obtained analytical condition of the onset of chaos. Further numerical calculations of nonlinear Hamiltonian chains [7, 8] confirmed these results.

Now the study of the chains which are in the contact with thermostat is of most interest. Dynamical properties of such systems are more complicated. They are not Hamiltonian ones and describe the open systems which can exchange energy with environment. The systems under uniform temperatures are of marginal interest. But the systems with nonuniform temperature are much more interesting because they provide the thermal transport from higher temperature to lower. Such systems are investigated intensively.

The different dynamical properties of different 1D chains result in various heat transport laws. The heat transfer in macroscopic solids obeys the Fourier heat conduction law

$$J = -k\nabla T, \quad (1)$$

where J is the heat flux, k is the thermal conductivity, which doesn't depend on a sample size, and ∇T is the temperature gradient.

Now the validity of the Fourier law is justified by means of numerical calculations in the ding-a-ling [9] and the Frenkel and Kontorova [10] models. The integrable systems, such as harmonic [11] and Toda [12] chains, don't

form the temperature gradient because there is no scattering of the thermal excitations which transport the heat. The thermal conductivity of these systems is divergent. The FPU chains [13–16], the diatomic Toda lattice [17], the Heisenberg spin chain [18] take intermediate states. The thermal conductivity of the models diverges as $k \sim N^\alpha$ at the number of particles $N \rightarrow \infty$ with $0 < \alpha < 1$.

In this paper we do not consider the thermal conductivity of chains with the large numbers of particles. We set sparser task which is to examine the dynamical behavior of short chains of the FPU type, which are in the contact with thermostates, and to compare them with that of similar Hamiltonian chains under suitable conditions.

II. HAMILTONIAN CHAINS

The dynamical properties of the systems with great number of the degrees of freedom are hard to investigate numerically. To avoid the problem we consider the atomic chains with small numbers of particles and assume that their characteristic properties can be extended to the chains with greater dimension.

As a model we used the 1D chain of N classical particles with mass m positioned in the points x_i and interacting with each other via a nonharmonic potential $U(x_{i+1} - x_i)$. In the equilibrium state the particles are located at equal distances a from each other. Dynamics of the chain obeys the classical equations of motion

$$m \frac{d^2 x_i}{dt^2} = -\frac{1}{2} \frac{d}{dx_i} [U(x_i - x_{i-1}) + U(x_{i+1} - x_i)], \quad (2)$$

where $i = 1..N$. Indexes $i = 0$ and $N + 1$ correspond to the motionless points with coordinates $x_0 = 0$ and $x_{N+1} = (N + 1)a$ which are the boundary conditions for Eq.(2). Potential used in the model is the sum of the harmonic and the quartic terms

$$U(x) = \frac{k}{2}x^2 + \frac{\beta}{4}x^4, \quad (3)$$

where k is the elasticity factor and β is the nonlinearity parameter.

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Hereinafter the model parameters used are $m = k = a = 1$ and $\beta = 2$. The system of the ordinary differential equations Eq.(2) was solved numerically by means of the modification [19] of the Verlet algorithm [20].

The randomly chosen particle velocities at the equilibrium particle positions were used as the initial conditions. The kinetic energy per particle, which we call "temperature", is used as driving parameter which controls the type of dynamics.

Now it is known that a nonlinear Hamiltonian particle chain with $N > 1$ can demonstrate a quasiperiodic or a chaotic type of motion. To identify the character of the chain motion we analyzed the time series, which are the sets of velocities of the second particle in a chain taken with the time interval $Dt = 1$. Such an approach is widely used to investigate the properties of chaotic systems [21]. The power spectrums and the autocorrelation functions of the solutions were the criteria of the chain dynamics. The examples of these functions corresponding to the 4-particle chain which is in a regular and a chaotic dynamical states in the close vicinity of the boundary temperature are shown in Figs.1 and 2.

An additional information was obtained by means of the calculation of the correlation dimension D_c which evaluates the lower limit of the Hausdorff dimension of the subset of the phase space occupied with the solutions. In the case of a quasiperiodic motion D_c gives the dimension of the corresponding invariant torus. In all cases examined $D_c = N$ for the regular dynamics. In the chaos regime the correlation dimension seemingly strongly depends on initial conditions and is a random value. Temperature dependence of the correlation dimension of the 4-particle chain solutions is plotted in Fig.3.

If these characteristics did not make it possible for identification of the type of motion unambiguously, the time behavior of phase trajectories with close initial conditions was analyzed.

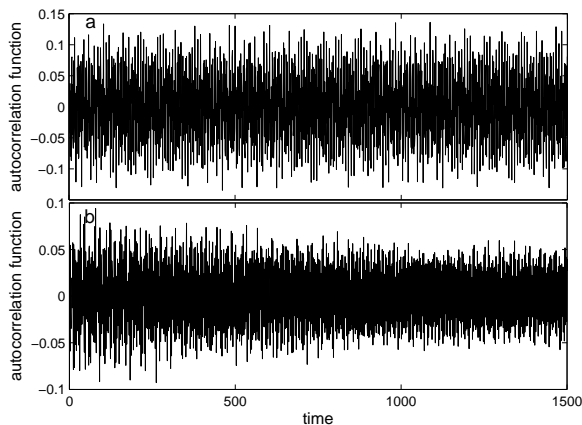


FIG. 1. Autocorrelation functions (a) of the quasiperiodic motion of 4-particle chain at $T = 0.131$ and (b) of the chaotic one at $T = 0.133$.

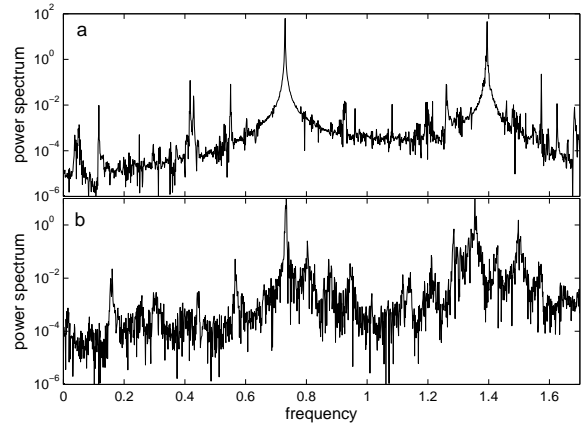


FIG. 2. Power spectrum (a) of the quasiperiodic motion of 4-particle chain at $T = 0.131$ and (b) of the chaotic one at $T = 0.133$.

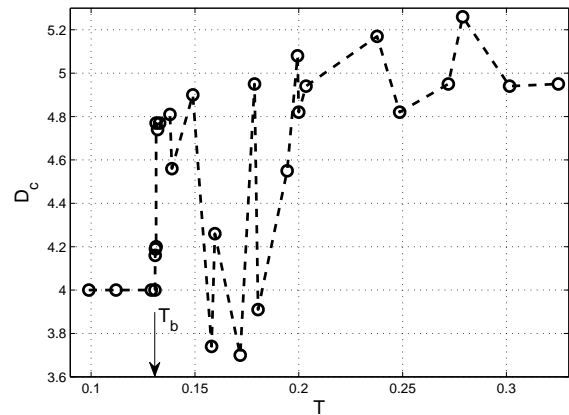


FIG. 3. Correlation dimension D_c versus temperature T for the 4-particle chain. The arrow points the boundary temperature between the regular and the chaotic motions

We examined the behavior of the chains with $N = 2 - 8, 10$ at different initial conditions in the regions of a regular and a chaotic motion to find the boundary temperature T_b between them. Results of the calculations are shown in Fig.4. The numerically obtained boundary temperatures are marked by open circles. These points separate the regions of a regular and a chaotic dynamics of the chains. The dependence obtained was fitted by the function $T_c = 2.28N^{-2.06}$ shown by the solid line. The numerical parameters were found by means of the least square method. This dependence is in qualitative accordance with the Chirikov criterion [6] which predicts that critical parameter $\epsilon_s \sim N^{-2}$ for large N and high modes.

There are two short chains ($N = 2, 3$) which fall out from the dependence discussed. Two-particle chain under reasonable restriction on temperature (particle shift $\Delta x \lesssim a$) demonstrates a regular dynamics only. In the case $N = 3$ $T_b \approx 0.965$ is considerably larger than that

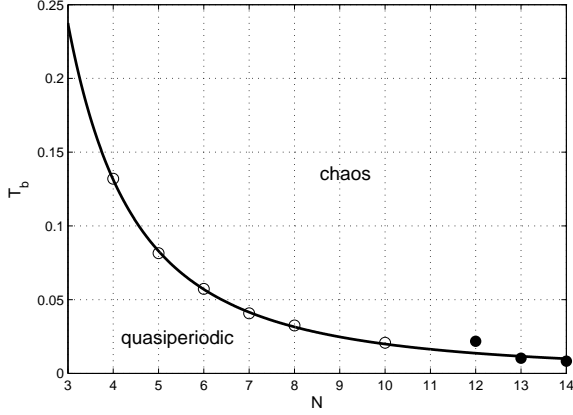


FIG. 4. Temperature T_b separating two types of dynamics as a function of the chain length N . Open circles show the boundary temperatures of the Hamiltonian chains. Line is the fitting curve which follows the dependence $T_b(N) = 2.28 \cdot N^{-2.06}$. The close circles show T_b of the thermostated chains.

in Fig.4.

As it follows from the obtained dependence, the boundary temperature T_b decreases rapidly when the chain length N grows. Moreover, the total boundary energy of the chains $E_N = NT_b$ decreases as N^{-1} .

III. THERMOSTATED CHAINS

In this section we consider the 1D atomic chains interacting with a thermostat, i.e. with a large system which is under constant temperature and isn't influenced by the chain. This problem is very different from that considered in the previous section.

The motion of the Hamiltonian chains is stipulated unambiguously by the initial conditions and the chain total energy is an integral of motion. In this case the system dynamical properties can be obtained by means of analyzing the phase trajectories or the time series.

An open system exchanges energy with a thermostat. In this case the system total energy is fluctuating. Other difference is that the dynamics and fluctuations of the system are driven by the same cause, that is the thermostat temperature. In this case the contributions of the dynamics and the fluctuations in the motion of the system are the same and we can't separate them.

In this section we consider the chains in which the first and the last particles are in the contact with the thermostats with temperatures T_1 and T_N . The thermostat temperatures are the parameters of the problem. We used both the Langevin and the N  se-Hoover [22] thermostats. Both of them give the qualitatively same results. Therefore we show the results obtained with the N  se-Hoover thermostat only.

First we considered the chains at the uniform temperature $T = T_1 = T_N$. To understand the chain behavior we

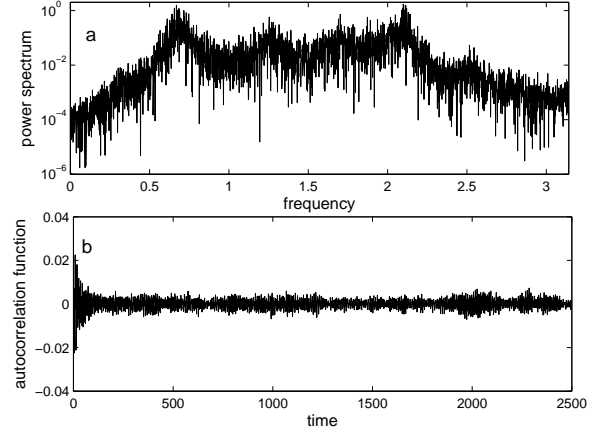


FIG. 5. Power spectrum (a) and autocorrelation function (b) of the 4-particle chain at the thermostat temperature $T = 0.05$.

analyzed the time series and plotted the autocorrelation functions and the power spectrums of the chains with different N and the thermostat temperatures T . The results for $N = 4$ and $T = 0.05$ are shown in Fig.5. As it is seen in Fig.4 this temperature corresponds to the quasiperiodic motion of the Hamiltonian chain. However, the plots Fig.5 are characteristic rather to noise with short correlation time than to a dynamical motion. Such a picture is typical for the chains with other N and at the temperatures regions corresponding to both a quasiperiodic and a chaotic motion.

Other approaches used in Section II also don't allow to identify a type of motion. The correlation dimensions are more than the total phase space one $D_c > 2N$ at any temperatures what doesn't correspond to either dynamical motion. The behavior of two phase trajectories with close initial conditions at any temperatures is typical to a developed chaos.

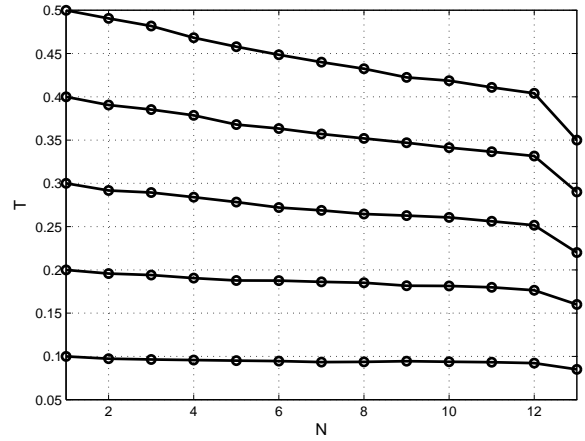


FIG. 6. Temperature profiles of the 13-particle chain.

But the study of the chains with a nonuniform temper-

ature distribution was more informative. We calculated the temperature distribution along the chains at different temperatures on left and right ends and plotted the temperature gradients as functions of temperature for different chains. The main difficulty in such an approach is that the temperature gradient at a fixed number of particles strongly depends on both temperatures. We tried to find the maximum temperature gradient which can be formed in each chain at given left temperature T_1 . The temperature profiles for the chain with $N = 13$ at left temperatures in the interval $T_1 = 0.1 - 0.5$ are plotted in Fig.6. To find the profile we specified the thermostat temperatures on the chain ends and waited during time interval $t = 10^4$ to thermalize the chain. Then we get the local temperature as a particle kinetic energy averaged over the time interval $t = 10^5$.

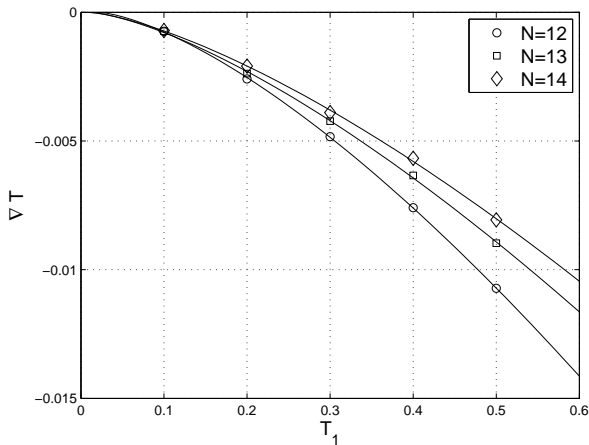


FIG. 7. Temperature gradient as function of temperature T_1 for the chains of different length.

The temperature gradients as the functions of the temperature of the first particle T_1 are shown in Fig.7 for the chains with $N = 12, 13, 14$. They were found by the least square method using $N - 1$ points of the chains with the exception of the last one. The markers show the points calculated. The solid lines fit the dependencies obtained using the expression

$$\nabla T = A(T_1 - T_b)^b. \quad (4)$$

The fitting parameters are shown in the Table. The parameter T_b is the temperature at which the temperature gradient becomes zero. At lower temperatures $T < T_b$ the temperature gradient is equal to zero.

N	T_b	A	b
12	0.0213	-0.0315	1.46
13	0.0103	-0.0248	1.43
14	0.0083	-0.0221	1.42

The heat flux is finite at any temperature T_1 if $\Delta T = T_1 - T_N$ is finite. Therefore the thermal conductivity

diverges as soon as $T_1 \rightarrow T_b + 0$ and it is divergent at $T < T_b$. This means that the interaction of the thermal excitations transferring the heat, which is responsible for the conductivity, disappears at this temperature. The thermal conductivity is plotted as the function of the temperature T_1 in Fig. 8.

The temperatures T_b of the thermostated chains are shown in Fig. 4 by the close circles. They lie in the close vicinity of the positions corresponding to the boundary temperatures T_b of the Hamiltonian chains with the same number of particles. These temperatures separate the regions of stochastic and the regular motion of the chains under thermal fluctuations. So, we can see analogy between the dynamics of the Hamiltonian and the thermostated chains.

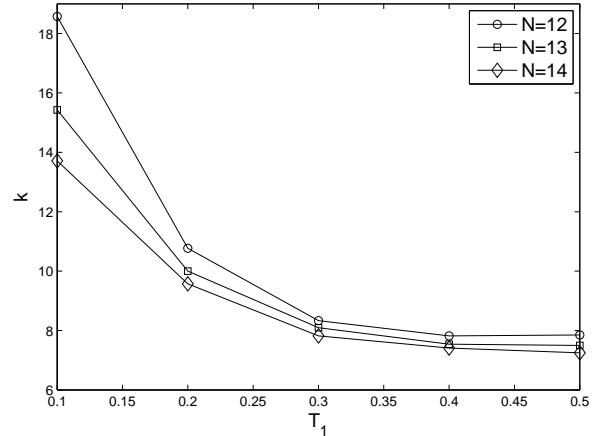


FIG. 8. Temperature dependence of the thermal conductivity for the chains of different length.

IV. CONCLUSION

We considered the dynamics of short Hamiltonian chains and chains interacting with the thermostats. It is shown that both types of the chains demonstrate similar dynamical behavior. In particular, the Hamiltonian chains depending on temperature can be in two dynamical states, regular (quasiperiodic) and stochastic (chaotic), which are separated by the boundary temperature T_b (Fig.4). The results were obtained by means of analyzing of time series.

This approach doesn't work in the case of the thermostated chains because of strong thermal fluctuations. In this case we used the indirect method to ascertain dynamics of the chains. We analyzed the temperature dependence of the slope of the temperature profiles of the chains and found the temperature T_b at which the slope vanishes. At the temperatures $T \leq T_b$ the thermal conductivity is divergent as it takes place in integrable systems. So, we can suppose that in this temperature interval the chain, in spite of the fluctuations, demonstrates

the regular (fluctuated quasiperiodic) motion. Accordingly, at $T > T_b$ the chain dynamics is stochastic (fluctuated chaotic).

The method used to analyze the thermostated chains allows us to evaluate the boundary temperatures only.

We can specify a regular or a stochastic chain motion but can't obtain its more detailed characteristics, which are responsible for the thermal conductivity behavior. Apparently, for this purpose investigation of the Hamiltonian chains is more promising.

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